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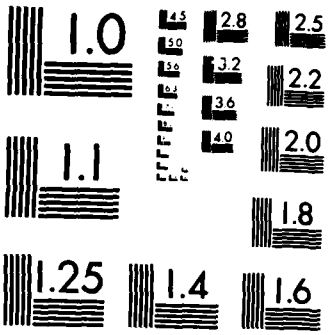

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TECHNICAL REPORT ARLCB-TR-84031

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APPLICATION OF THE DIFFRACTION MODEL TO AMORPHOUS MAGNESIUM ZINC ALLOYS

P. J. COTE
L.V. MEISEL

OCTOBER 1984

US ARMY ARMAMENT RESEARCH AND DEVELOPMENT CENTER
LARGE CALIBER WEAPON SYSTEMS LABORATORY
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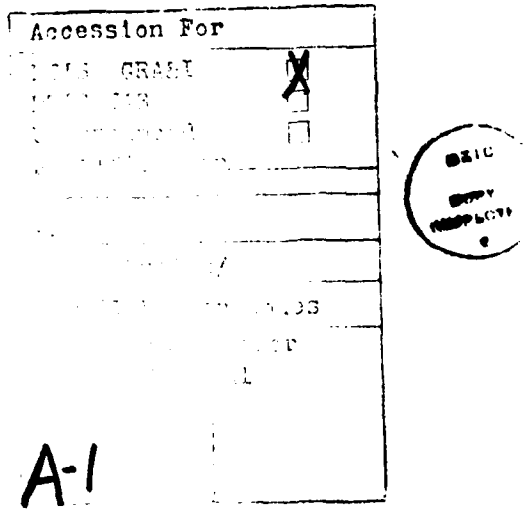
TABLE OF CONTENTS

LIST OF ILLUSTRATIONS



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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Amorphous magnesium-zinc (a-MgZn) alloys comprise the best system available for testing the diffraction model for electron transport in non-crystalline alloys. They are simple metal binary alloys. Conventional methods exist for determining electronic parameters in the model. They exhibit low resistivities so that saturation effects are not expected to dominate. They are well characterized and extensive resistivity data are available.

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20. ABSTRACT (CONT'D)

Computed results presented here are based on a refinement of previous calculations; the alloy scattering matrix elements with computed phase shifts for Mg and Zn are used with the substitutional model instead of the adjusted effective potential assumed previously. Results obtained ignoring mean free path effects are in qualitative agreement with the data; agreement is surprisingly detailed when account is taken of saturation effects.

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INTRODUCTION

In a recent paper (ref 1) we presented quantitative results of diffraction model (ref 2) calculations of the temperature dependence of the resistivity of amorphous magnesium zinc (a-MgZn). The phase shift expansion of the scattering matrix elements as derived by Evans et al (ref 3) was used with the phase shifts adjusted to give the observed magnitude of the resistivity and to satisfy the Friedel sum rule. Saturation effects (ref 4) were included by invoking the Pippard-Ziman mean free path constraint (refs 1,2,5) on the electron-phonon interaction. A single effective scattering potential was used in place of the full alloy scattering matrix elements. Comparison of these computed results with the data of Matsuda and Mizutani (ref 6) in a-MgZn showed remarkable agreement between theory and experiment on all the many features of the temperature dependence of the resistivity. It was therefore considered worthwhile to refine the calculations by using the alloy scattering matrix elements with phase shifts computed for Mg and Zn in an extended version (ref 7) of the Ziman-Faber substitutional model (ref 8). Selected results pertaining to a-MgZn are presented here. Additional results relating to low resistivity alloys in general are given in Reference 9.

THEORETICAL MODELS

We employ a form (ref 7) of the Ziman-Faber liquid alloy substitutional model (ref 8) which is appropriate for an amorphous Debye solid (ref 10). The result for the electrical resistivity is

$$\rho = \frac{12\,\Omega_o}{e^2 h V_F^2} \int_0^1 d\left(\frac{K}{2k_F}\right)\left(\frac{K}{2k_F}\right)^3 |U(K)|^2 \qquad (1)$$

References are listed at the end of this report.

where

$$|U(K)|^2 = c_1c_2|t_1(K) - t_2(K)|^2 I^{\rho}(K)$$
$$+ |c_1t_1(K) + c_2t_2(K)|^2 S^{\rho}(K) \qquad (2)$$

and c_i and $t_i(K)$ are the concentration and t-matrix for the i^{th} component. The resistivity structure factor is given by

$$S^{\rho}(K) = e^{-2W(K)}a(K) +$$

$$+ \frac{\alpha\theta_R}{T}\left(\frac{K}{2k_F}\right)^2 \int_0^1 d\left(\frac{q}{q_D}\right)\left(\frac{q}{q_D}\right)^2 n(x)(n(x)+1)F(q\Lambda) \int_0^1 \frac{d\Omega_q}{4\pi}\, a(\vec{K}+\vec{q}) \qquad (3)$$

where $\alpha = 3(2hk_F)^2/Mk_B\theta_R$.

The corresponding cross term integral is given as

$$I^{\rho}(K) = e^{-2W(K)} + \frac{\alpha\theta_R}{T}\left(\frac{K}{2k_F}\right)^2 \int_0^1 d\left(\frac{q}{q_D}\right)\left(\frac{q}{q_D}\right)^2 n(x)[n(x)+1]F(q\Lambda) \qquad (4)$$

The partial geometric structure factors in the substitutional models are assumed to be identical and are given by

$$a(K) = \frac{1}{N}\sum_{m,n} \exp[i\vec{K}.(\vec{m}-\vec{n})] \qquad (5)$$

where m and n represent the average ion positions.

The scattering matrix elements for the i^{th} component is given by

$$t_j(K) = \frac{2\pi h^3}{m(2mE_F)^{1/2}\Omega_o} \sum (2\ell+1)\sin \eta_\ell{}^j(E_F)\, e^{i\eta_\ell{}^j(E_F)} P_\ell(\cos\theta) \qquad (6)$$

where $\eta_\ell{}^j(E_F)$ are the scattering phase shifts.

The Pippard-Ziman constraint (ref 5) on the electron-phonon interaction reflects the breakdown of the adiabatic approximation due to finite electron mean free paths Λ and is incorporated here through the Pippard function (ref 11) $F(q\Lambda)$ where

$$F(y) = \frac{2}{\pi}\left[\frac{y \tan^{-1} y}{y - \tan^{-1} y} - \frac{3}{y}\right] \qquad (7)$$

In the long mean free path limit $F(q\Lambda) \to 1$ and the above expressions reduce to standard diffraction model results.

The remaining terms in the above expressions have their usual meaning; other details and definitions are given in Reference 9.

RESULTS AND DISCUSSION

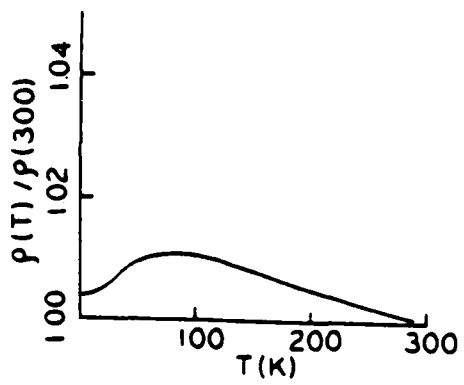
The phase shifts for these calculations were obtained by constructing muffin tin potentials with the Mattheiss prescription (ref 12) using Herman and Skillman (ref 13) neutral atom wave functions. For Mg the Kmetko (ref 14) value of 0.75 of full Slater exchange was used. For Zn the value of 0.85 of full Slater exchange was used since this places the d-levels at approximately 9 eV below E_F, which is appropriate for Zn alloys. The phase shift values were then computed using modified versions of computer routines given by Loucks (ref 15). The $\ell = 0$ to $\ell = 3$ values at E_F in the 72 percent Mg alloy for Mg are -0.175, 0.085, 0.034, and 0.001, respectively. For Zn the corresponding values are 0.354, 0.294, -0.057, and 0.002.

The other parameters used in the computations were based on the following: x-ray data (ref 16) for a-Mg_7Zn_3 show the main peak in the structure factor is located at $k_p = 2.7\text{Å}^{-1}$ for the a-MgZn composition range. We assume that k_p varies so that $2k_F/k_p = 1.11$ is appropriate for the composition range; the average ionic mass was used for M; a Debye phonon spectrum is assumed and, since $z \approx 2$, we took $q_D = k_F$; specific heat data (ref 17) give $\theta_D = 295$K for the low temperature limit, but we selected $\theta_R =$

200K for the resistivity Debye temperature to fit the room temperature TCR. (For crystalline Mg, θ_D = 390K and θ_R = 340K, while for Zn, θ_D = 310K and θ_R = 175K (ref 18).) A geometric structure factor of Percus-Yevick form with packing fraction of 0.525 is appropriate for amorphous alloys (ref 18) and was used here.

Detailed experimental data for a-$Mg_{1-x}Zn_x$ for $.225 \leq x \leq .325$ were obtained by Matsuda and Mizutani (ref 6). All compositions show negative TCR's at the high temperatures and resistivity maxima ranging between 40 to 60K; most also show broad shallow minima centered at approximately 10K. Another feature found by Matsuda and Mizutani is that the resistivity varies as $(T-T_M)^{3/2}$ for $T > T_M$, where T_M is the temperature at the resistivity maximum.

The results of the present calculation are shown in Figures 1 and 2. The computed magnitude of ρ is about 40 $\mu\Omega$cm. In Figure 1 we see the ρ vs. T behavior computed from the standard diffraction model (Eqs. (1) through (7) with $F(q\Lambda) = 1$): a maximum and a negative TCR at room temperature are obtained in the calculation, however, T_M is higher than observed by about a factor of two, the calculated magnitude of the TCR at room temperature is too small by at least a factor of four, and the size of the maximum is too large by two orders of magnitude. The low temperature T^2 limit occurring in the standard diffraction model, (i.e., $\rho = \rho_o(1+BT^2)$ with $B \cong 3\times10^{-6}K^{-2}$) holds up to about 15K. This is not consistent with the data either since the mean value for B obtained by Matsuda and Mizutani (ref 6) is $0.5 \times 10^{-6}K^{-2}$ and the temperature range for this approximate quadratic dependence is considerably extended.



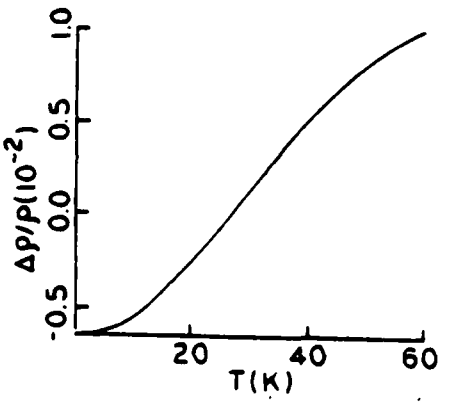


Figure 1. Resistivity vs. temperature curves for 32.5% Zn composition. $\Delta\rho = \rho(T) - \rho(300)$; no saturation.

Figure 2 shows the result with saturation effects included. The value of $q_D\Lambda$ was set at 11.6 to correspond to the observed ρ value at $x = .325$ and to a saturation resistivity of 200 $\mu\Omega$cm. The previous calculations (ref 1) with the effective potential approximation, including saturation, reproduced many of the observed features such as the presence of minima, the correct magnitude and approximate average position of the maxima, the $(T-T_M)^{3/2}$ dependence, and the reduced magnitude of B. The present results show these features: for example, the value of B for $x = .325$ is approximately $0.5 \times 10^{-6}K^{-2}$ with an extended T^2 range. In addition, the observed shape and position of the minima are obtained; the trends in size and position of the minimum and maximum in resistivity and the magnitude of the resistivity are also consistent with th data.

CONCLUSIONS

The results underscore the point that effects of finite electron mean free paths are important in the temperature dependence of the resistivity of amorphous alloys, even in alloys with resistivities as low as 50 $\mu\Omega$cm. Only qualitative agreement with experiment is obtained if saturation is ignored. Earlier work (ref 2) showed that not even qualitative agreement with the diffraction model could be obtained at higher resistivities unless these effects are considered. The detailed agreement between the present computations, which include saturation, and the many features of the ρ vs. T data of a-MgZn is remarkable.

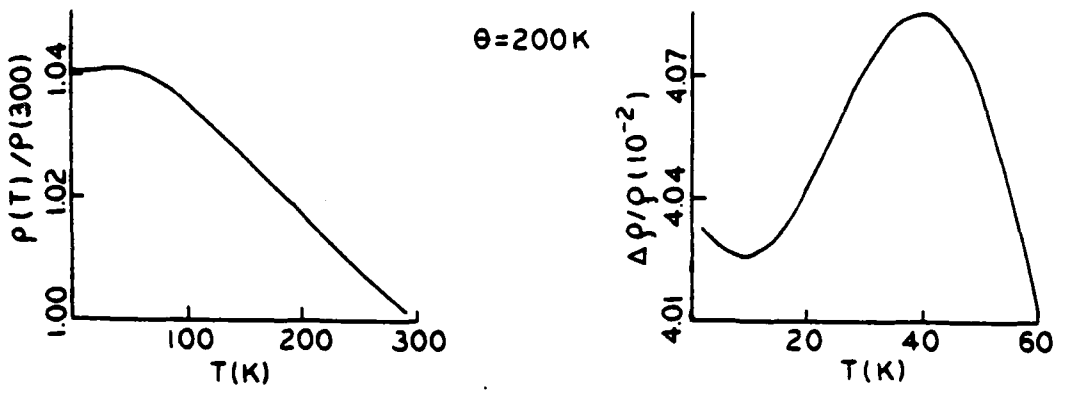


Figure 2. Resistivity vs. temperature for 32.5% Zn composition. $\Delta\rho = \rho(T) - \rho(300)$; $q_D\lambda = 11.6$.

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